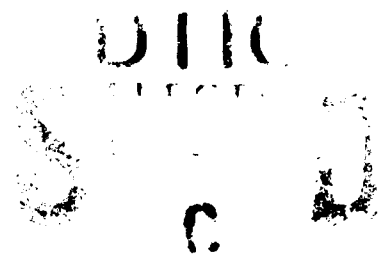


AD-A243 359



FINAL REPORT



Contract N00014-89-K-2021

EQUATION OF STATE AND CONDUCTIVITY OF
HOT, DENSE MATTER

Gabor J. Kalman

Principal Investigator

Department of Physics

Boston College

Chestnut Hill, MA 02167

Period covered:
April 15, 1989 through December 31, 1990

Approved for release
Distribution Unlimited

91 11 21 10 13

91-16492



I. OBJECTIVES

The purpose of the research program reported there was to develop and apply a novel method to the calculation of the Equation of State (EOS), Mean Charge State (MCS) (or degree of ionization) and conductivity of dense plasmas of moderately high Z-numbers ($Z < 30$). The method to be applied was the Thomas-Fermi model, modified and adapted to the dense plasma environment by the author and Ying [1]. The innovative elements of the approach are:

- 1) The plasma environment is represented by the ion-ion and ion-electron correlation functions as source densities in the TF equation.
- 2) The bound electron density is posited to be zero at the ion boundary: this gives a reasonably defined ion radius, separates free and bound electrons and eliminates both the unphysical extra pressure due to bound electrons (characteristic to the so-called "Confined Atom" model) and the infinite ion radius (characteristic to the TF - Debye model).
- 3) The MCS is determined by minimizing the free energy (F) of the combined TF-ion/plasma system, with the proper inclusion of all electron-electron, electron-ion, ion-ion correlations.
- 4) The method can be combined with the approach of Davis and Blaha, who solved the exact Schrodinger equation for the valence electron in the TF-potential of the core electrons.

The original program was formulated for a three-year period, and was planned to be funded on an appropriate level. In fact, after the exploratory funding of the first year, the planned second year funding was drastically reduced and third year completely eliminated. Consequently only a limited portion of the original objectives have been achieved.

II. ACCOMPLISHMENTS

1. In order to obtain a reliable description of the correlations, a hypernetted chain (HNC) integral equation has been developed for the system. The interaction potential between the ions is properly determined by the combined charge of the nucleus and the bound electrons.

but does not include the effect of the penetrating free charges. The free electron-ion interaction is represented by an effective potential which phenomenologically includes the softening quantum - effects near $\mu = 0$ and the effects of exchange with the bound electrons. [2,3] The two component HNC code has been developed and has been tested against the existing HNC computer code for pure Coulomb system, developed by the Livermore group [4].

2. The HNC and TF equations become coupled because interaction potential depends on the bound electron distribution, which, in turn, is affected by the correlations between the selected ion and its surroundings. A corresponding TF-HNC computer has been developed.

3. In order to determine the free energy of the plasma without the cumbersome and unreliable standard temperature integration, we have adopted the method of Hill [5], which requires space integrals over the pair correlation functions only.

4. We have solved the combined TF-HNC-F code for $Z = 6$ (Carbon), $Z = 13$ (Aluminum) and $Z = 29$ (Copper) for a wide range of temperature and density values:

$$T = 1, 10, 20, 50, 100, 200, 500, 1000 \text{ eV}$$

$$m = 10^{19}, 10^{20}, 10^{21}, 10^{22}, 10^{23}, 10^{24}, 10^{25}, 10^{26} \text{ cm}^{-3}$$

and determined the following quantities:

- A. MCS (z):
- (i) $z(T; n, Z)$
 - (ii) $z(n; T, Z)$
 - (iii) equi-z contours in the (n,T) plane

- B. Correlation functions $g_{AB}(r)$:
- (i) $g_{\text{ion-ion}}(r)$
 - (ii) $g_{\text{ion-electron}}(r)$
 - (iii) $g_{\text{electron-electron}}(r)$

- C. Static structure functions $S_{AB}(k)$
- (i) $S_{\text{ion-ion}}(k)$
 - (ii) $S_{\text{ion-electron}}(k)$
 - (iii) $S_{\text{electron-electron}}(k)$
 - (iv) $S_{\text{charge}}(k)$

Statement A per telecon
Murray Bradley
NRL/ Code 20375
NW 12/12/91

A-1

D. EOS: $P(n; T, Z)$ (pressure)
 $E(n; T, Z)$ (energy)
 $F(n; T, Z)$ (free energy)

E. Energies of the bound electrons:
 $E_{\text{bound}}(z; Z, n, T)$

and "ionization energies"

$$I_z(Z; n, T) = E_{\text{bound}}(z - 1; Z, n, T) - E_{\text{bound}}(z; Z, n, T)$$

Note that the ionization energies here are explicit functions of n and T .

5. We have compared our results with results available in the literature on the MCS and on the EOS: they include Davis and Blaha [6], More [7] Fen et. al. [8], the Los Alamos SESAME Code, Foster et. al. [9] Latter [10] and Soviet data provided by Professor E. Son. [11]. The results are free from the usual anomalies plaguing TF calculations, approach the Saha equation results for low densities and correctly portray pressure ionization effects at high densities.

6. In summary, we have developed a unique model, applicable over a wide range of density and temperature values for medium or high Z plasmas, which, we contend, represents the most reliable approach to hot, dense plasma MCS calculations.

7. In view of the availability of effective "ionization energies" (see above), it has become possible to abandon the average atom picture inherent in the present calculations and replace it with a Saha-like equation which can correctly describe fluctuations and integer z -numbers and describes the system in terms of integer z values only.

REFERENCES

1. R. Ying and G. Kalman, Proc., XVIII Int. Conf. on Phenomena in Ionized Gases, ed. by W. T. Williams, (1987). R. Ying and G. Kalman in Strongly Coupled Plasma Phys. ed. by F. J. Rogers and H. E. DeWitt (1986). R. Ying and G. Kalman Thomas-Fermi Model for Dense Plasma, Phys. Rev. **A40**, 3927(1989).
2. T. Dunn and A. Broyles, Phys. Rev. **157**, 156(1967).
3. F. J. Rogers, Phys. Rev. **A29**, 868(1983).
4. F. J. Rogers, private communication.
5. T. L. Hill, Statistical Mechanics (McGraw- Hill, New York, 1956).
6. J. Davis and M. Blaha, Atomic Processes in Plasmas, Gaithersburg MD, October 1989.
7. R. M. More, in Applied Atomic Collision Physics, edited by H. S. Massey (Academic, New York, 1983), Vol. 11.
8. I. J. Feng, W. Zakowicz, and R. H. Pratt, Phys. Rev. A **23**, 883 (1981).
9. A. Foster et al. XXth Int. Conf. on Phenomena in Ionized Gases, Pisa, Italy, July 1991.
10. R. Latter, Phys. Rev. **99**, 1854 (1955). R. Latter, J. Chem. Phys. **26**, 270 (1956).

III. PUBLICATIONS AND PRESENTATIONS

1. R. Ying and G. Kalman Model for Dense Plasma, Phys. Rev. **A40**, 3927 (1989).
2. G. Zhou and G. Kalman, Atomic Processes in Plasmas Gaithersburg, MD, October 1989.
3. G. Kalman: New Thomas-Fermi Model, Inst. Theor. Phys., Santa Barbara CA, December 1989.
4. G. Kalman, SDIO Program Review, Alexandria, VA, October 1990.
5. G. Zhou and G. Kalman: Thomas Fermi- HNC Calculations of the Degree of Ionization in Dense Plasmas, XXth Int. Conf. on Phenomena in Ionized Gases, Pisa, Italy, July 1991.

6. G. Zhou and G. Kalman: HNC Calculations for the Correlated Thomas-Fermi Model for Dense Plasmas., Atomic Processes in Plasmas, Portland MA, August 1991.
7. G. Zhou and G. Kalman: Thomas - Fermi HNC Model for Dense Plasmas, Int. Workshop on Nonideal Plasmas, Berlin, Germany, November 1991.

(a)GK